Title: Safety Applications Project FY20-21 Highlights, FY22 Goals

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Los Alamos
NATIONAL LABORATORY

Safety Applications Project
FY20-21 Highlights, FY22 Goals

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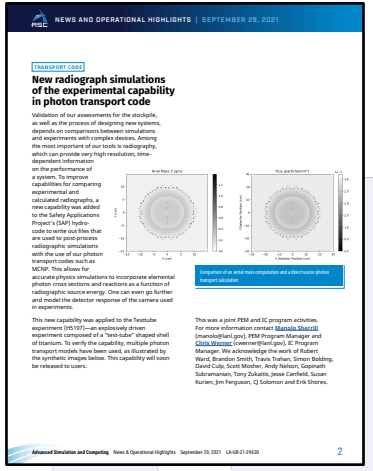
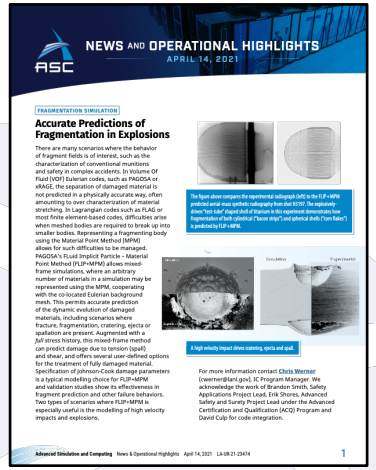
Outline

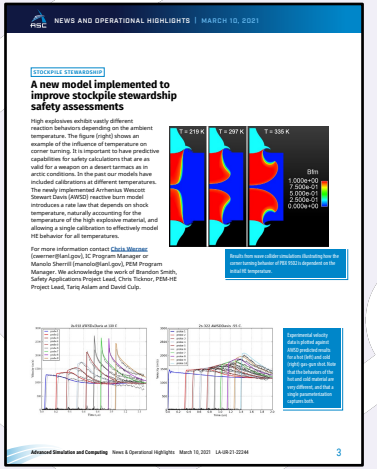
- Highlights
- Collaborations
- Capabilities
- Infrastructure
- Performance

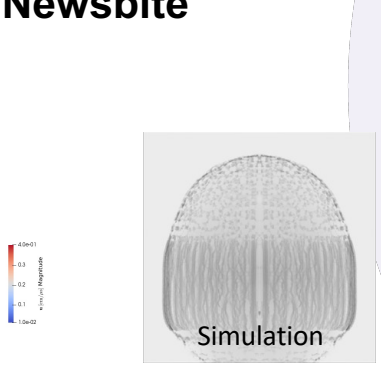
FY20-21 Highlights

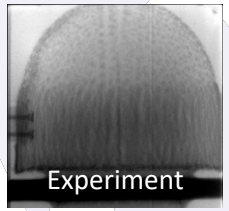
- Mark & Emily joined team
- March 2021: AWSD Newsbite
- April 2021: FLIP+MPM Newsbite
- August 2021: Sierra L2 Milestone
- August 2021: LAAP award for infrastructure modernization
- September 2021: Talos Newsbite











Collaborations leverage the investment and expertise of others.

- PEM HE: reactive flow models, non-standard HE scenarios, mesoscale HE
- PEM TR: EnSight output, Talos output
- CSSE Production Visualization: ParaView output
- JMP: lagrangian particle hydrodynamics, non-standard HE scenarios, mesoscale HE
- ACQ: lagrangian particle hydrodynamics
- EM: performance improvement
- GS: targeted code needs
- …
- **Leveraging these funds has allowed meaningful improvement in 3D code performance and successful deployment of focused, unique code capabilities.**

Collaboration is key to advancing our simulation tools.

Code capabilities determine the questions that can be addressed using SAP tools.

Past: FY20-21

- AWSD reactive burn
- PiSURF
- 2D PDV
- 2D synthetic radiograph
- Talos output
- Significant memory reduction of a package
- JWLB for overdriven HE
- Improved initialization, EOS and MATCH temperature support
- Sparse material numbering and improved body naming

Present: FY22

- rDSD
- PDV robustness
- Full ParaView support
- Viscoelastic brittle failure
- MATCH thermal ignition
- Affine transforms for analysis

Future

- Implicit hydro and H-S reaction networks
- Memory-efficient STL
- Automatic material priorities
- Gap opening
- Eulerian slidelines
- Improved ceramic and glass models

Tasks are determined by user needs, staff skills, resources, and programmatic constraints.

Infrastructure acts as a force multiplier for software developer skills.

Past: FY20-21

- ATS-2 nightly testing
- ATS-2 NVHPC nightly build
- Spack environments
- Compiler warnings
- Resolve test diffs
- Finish LaTeX docs
- Git/GitLab migration
- Perl to Python conversion
- Modularize source files

Present: FY22

- CMake
- GitLab CI on HPC
- Production-level Sierra support

Future

- Container builds

Paying down infrastructure debt is complete.

Improved code performance allows simulations to finish faster or with greater fidelity.

Past: FY20-21

- Pre-inverted EOSPAC
- Turn off EOSPAC extrapolation check
- Parallel EnSight output
- Inline Gen
- Automated restart
- Partial GPU support
- Code releases on ATS-2
- Turquoise deployment for DoD
- Remove sync points from EOS evaluation

Present: FY22

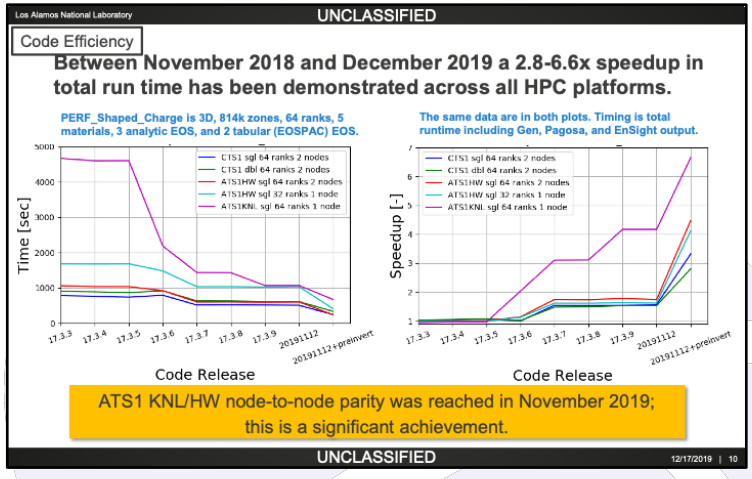
- Profiling and optimization
- Robustness at resolution
- Relax Intel FP model
- Improved interface efficiency to analysis packages
- HDF5 restart

Future

- Ray-trace Calico
- Vectorization improvements
- Full GPU port
- Flexible mesh management

Implementation, testing, documentation, and user support are not called out—these are our everyday job.

Code performance has dramatically improved over the past ~4 years.



- Performance improvement is an ongoing priority.
- Significant gains have been achieved through vectorization, targeted optimization, improved modeling choices, and removal of synchronization points.
- User-relevant 3D simulations on CTS-1 resources finish in less than a day.
  - 1000 μm & 40 nodes: After 5-9x speedup these simulations finish in 1 hour.
  - 500 μm & 100 nodes: After another ~3x speedup these simulations finish in ~2 hours.
  - 250 μm & 100 nodes: In progress…

3D 500 μm benchmark simulation exercised since 2018 is 24% faster in FY21 and a combined 3.4x faster over FY20-FY21. 14% of FY21's improvement is due to avoiding EOSPAC's costly extrapolation check.